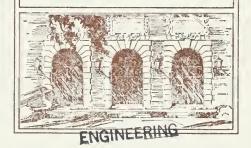


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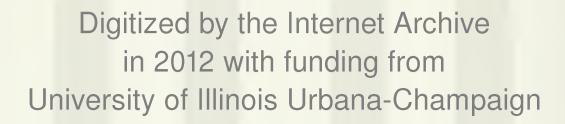
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THE QR-ALGORITHM

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Masako Ogura

September 1, 1971



THE QR-ALGORITHM

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ABSTRACT

The implementation of QR-algorithm on ILLIAC IV is described. An ASK subroutine for computing all eigenvalues of a real Hessenberg matrix of order less than or equal to 64 by this algorithm is attached. The QR-transformation consists of the decomposition of the matrix A_k into the product of a unitary matrix Q_k and an upper triangular matrix R_k , and forming A_{k+1} by post-multiplying R_k by Q_k , where A_1 = A is the original matrix. All eigenvalues are either isolated on the diagonal or are eigenvalues of a 2 x 2 diagonal submatrix as $k \to \infty$.



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1. INTRODUCTION

An ASK program for finding all eigenvalues of a real Hessenberg matrix of order less than or equal to 64 is written and tested on the B5500 simulator. The QR-algorithm for real Hessenberg matrices described herein is that of Martin et al [2]. The ILLIAC IV computer time required for performing one iteration (computation of A_{k+2} from A_k , refer to 4.1) on a 64 x 64 matrix is approximately 10 millisecond.

The necessary information for using this program is given in Section 2. The test result of this program on a 4×4 real Hessenberg matrix is given in Section 3. In Section 4, the outline of the QR-algorithm is given and Section 5 is devoted to the actual programming technique to implement this algorithm on the ILLIAC TV computer. The flow chart and ASK program are attached as Appendices 1 and 2 respectively.

This program assumes that the given real Hessenberg matrix is stored in the core memory in the straight storage scheme so that each row is stored across the PE's, starting with PEO. The real and imaginary parts of the eigenvalues found are to be stored in the two rows in the PE memory specified by the user. The original matrix is destroyed and replaced by the matrix which results from the QR transformations. The content of ACAR2 and ACAR3 are destroyed since the ACAR3 is used for linkage between the subroutine and main program and ACAR2 is used for passing the address of parameters to the subroutine.

2.1 Calling sequence

Calling sequence for this subroutine is:

CALL HQR (N, A, WR, WI, IT)

where A designates the first row of the matrix and is declared in the main program as

A: DATA
$$a_{00}, a_{01}, \dots, a_{0,N-1}, (0.0)M,$$

$$a_{10}, a_{11}, \dots, a_{1,N-1}, (0.0)M,$$

$$\dots$$

$$a_{N-1}, 0, a_{N-1}, 1, \dots, a_{N-1}, N-1, (0.0)M;$$
where $M = 64 - N$.

N is the size of the matrix declared as

N: EQU 64:

or

DEFINE N = 64 #;

or given as an integer, i.e., 64.

WR and WI are the rows in the PE memory where resulting real and imaginary parts of the eigenvalues respectively are to be stored. They are declared as

WR: BLK 1; and WI: BLK 1;

IT is the row vector in memory to which the number of iterations required for finding each eigenvalue is to be placed. This is declared as

IT: BLK 1;

If zero is placed in place of IT, it is to be considered that a user does not want to know the number of iterations required. The CALL macro should be defined in the user's program as:

```
DEFINE CALL &NAME (&PARAMETERS) =

&IF &SIGN (&MFIELD(&NAME))

&THEN EXTERNAL &NAME; &FI

&IF &EMPTY (&PARAMETERS) &THEN &ELSE

BEGIN BLOCK

BEGIN USE (63)

LIST: DATA & PARAMETERS

END;

CLC(2);

SLIT(2) LIST;

END; &FI

CLC(3);

SLIT(3) &NAME;

EXCHL(3) &ICR ##;
```

2.2 Core storage used

This routine uses 500 words of PE memory for storing instructions. One row is used for storing PE numbers and three additional rows are used for temporary storage. ADBO \sim 32 are also used.

2.3 Constant

EPS (ϵ), the constant which is used to test the convergence (4.1), is taken as 10^{-10} in this program. If a user wants to change the value of this constant, he may insert EPS: DATA (desirable value); in place of EPS: DATA @ - 10;

3. EXAMPLE

A test of this program was made on the B5500 simulator for the matrix:

with $\epsilon=10^{-8}$. The comparison of the eigenvalues obtained by this program to the exact values is given in Table 1. The selection of this small matrix and a relatively large ϵ was made because of the speed of the SSK simulator on the B5500; the execution speed ratio of the simulator to the ILLIAC IV is approximately 1:10⁶.

Table 1

Eignevalues obtained on B5500 simulator	Exact eigenvalues
3.99999997867	4.0
1.00000001066 + 1.999999999928i	1.0 + 2.0i
1.000000001066 - 1.999999999928i	1.0 - 2.0i
-1.000000000000	-1.0

4. QR-ALGORITHM

4.1 Brief outline of the QR-algorithm

The QR-transformation consists of the decomposition of the matrix A_k into the product of a unitary matrix Q_k and an upper triangular matrix R_k , and forming A_{k+1} by post-multiplying R_k by Q_k . Thus

$$A_{k+1} = R_k Q_k$$
 where $A_k = Q_k R_k$, (1)

therefore

$$A_{k+1} = Q_k^* A_k Q_k$$

where $A_1 = A$ is the original matrix. It can be shown in general that A_k tends to a form in which a_{i+1} , i a_{i+2} , i+1=0 for $i=0,1,\ldots,N-3$ as k increases. All eigenvalues are therefore either isolated on the diagonal or they are eigenvalues of a 2 x 2 diagonal submatrix. The amount of calculations involved in a QR step is greatly reduced if the matrix A is in the Hessenberg (or almost triangular) form. Since there are several stable methods available to reduce a general matrix to this form (ASK program HSBG is written for this purpose), the QR-algorithm is used after such reduction.

In order to achieve rapid convergence, it is essential that the origin shifts be applied and that each shift be close to an eigenvalue of the matrix. The QR-algorithm with shift of an origin \mathbf{s}_k is expressed as:

$$A_{k+1} = R_k Q_k + s_k I \qquad \text{where} \qquad A_k - s_k I = Q_k R_k$$
 (2)

or in other words

$$A_{k+1} = Q_k^* A_k Q_k$$

However, even when A_1 is real, some of the eigenvalues may be complex. If the transformation (2) is carried out with a complex value of s_k , A_{k+1} is in general a complex matrix. This deficiency can be overcome by performing two steps of (2) with shifts of s_k and s_{k+1} respectively. Since s_k and s_{k+1} are both real or complex conjugate in this transformation, A_{k+2} should be always real. This transformation is described as

$$A_{k+2} = Q_{k+1}^* Q_{k}^* A_{k} Q_{k+1}$$
and
$$(Q_{k} Q_{k+1}) (R_{k+1} R_{k}) = (A_{k} - S_{k}I) (A_{k} - S_{k+1}I)$$
(3)

One method of calculating A_{k+2} by (3) would be to form the real matrix $\Gamma = (A_k - s_k I) \ (A_k - s_{k+1} I)$, computing its unitary-triangular decompositon to obtain $Q_k \ Q_{k+1}$ and transform A_k by means of this, thus giving A_{k+2} . This process requires a prohibitive amount of work, but it is shown [1] that when the matrix is in the Hessenberg form, it is unnecessary to compute more than the first column of Γ , and that this immediately gives the transformation to be applied to A_k .

4.2 Practical computation

If (3) is rewritten as
$${\rm A_{k + 2}} = {\rm W^*A_kW} \qquad {\rm and} \qquad {\rm W^*\Gamma} = \Delta$$

where W = \mathbb{Q}_k \mathbb{Q}_{k+1} and Δ is the triangular matrix \mathbb{R}_{k+1} \mathbb{R}_k , W* is a unitary matrix which reduced Γ to the triangular Δ , and W is composed of N unitary factors of the form $\mathbb{M}_i = \begin{bmatrix} \mathbb{I}_i & -1 & 0 \\ 0 & \mathbb{B}_i \end{bmatrix}$ so that W = \mathbb{M}_1 \mathbb{M}_2 \mathbb{M}_k . From the form of each \mathbb{M}_i we see that the first column of W is equal to the first column of \mathbb{M}_1 , and this is any unitary matrix, the transpose of which eliminates the elements of the first column of Γ below diagonal.

Since we wish to transform A_k to A_{k+2} by W, we first operate on A_k with M_1 . This will change the first three rows and columns of A_k since the first column of Γ contains only three non-zero elements. It follows;

$$A_{k} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & \cdots & a_{0,N-1} \\ a_{10} & a_{11} & a_{12} & \cdots & a_{1,N-1} \\ & a_{21} & a_{22} & \cdots & a_{2,N-1} \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} \frac{a_{00}}{a_{10}} & \frac{a_{01}}{a_{11}} & \frac{a_{02}}{a_{22}} & \frac{a_{03}}{a_{23}} & \cdots & \frac{a_{0,N-1}}{a_{1,N-1}} \\ \frac{a_{10}}{a_{30}} & \frac{a_{11}}{a_{31}} & \frac{a_{12}}{a_{22}} & \frac{a_{23}}{a_{23}} & \cdots & \frac{a_{2,N-1}}{a_{3,N-1}} \\ \frac{a_{20}}{a_{30}} & \frac{a_{31}}{a_{31}} & \frac{a_{32}}{a_{32}} & \frac{a_{33}}{a_{33}} & \cdots & \frac{a_{3,N-1}}{a_{4,N-1}} \end{bmatrix}$$

where the elements changed by the row and column operations are underlined and primed respectively. The resulting matrix is no longer in the Hessenberg form and since A_{k+2} is in the Hessenberg form, we can say that the matrices $M_2 \cdot M_3 \cdot \cdot \cdot \cdot M_N$ reduce $M_1^* A_k^{-1}$ to the Hessenberg form. In the practical computation, therefore, it is necessary to compute only the first column of Γ .

a_N - 1, N - 1

After each iteration (we call the calculation of A_{k+2} from A_k an iteration), all subdiagonal elements of A_{k+2} are examined to see if any of them are "negligibly small." If so, the eigenproblem for the current matrix splits into that for two or more Hessenberg matrices of smaller sizes, and the iterations continue with the submatrix in the bottom right-hand corner. It may happen that while no individual subdiagonal element is sufficiently small to be regarded as negligible, the product of two consecutive elements may be small enough to permit us to work with a submatrix. Therefore the examination of the matrix A_{k+2} is performed to see if any two consecutive subdiagonal elements are small.

5. PROGRAM DESCRIPTION

5.1 Search for negligible subdiagonal elements

We assume that the size of the matrix under consideration is $(n+1) \times (n+1)$ where n takes integer values between 1 and N - 1. If the last negligible subdiagonal element is in position $(\ell, \ell-1)$, it is required only to work on the submatrix in the rows and columns ℓ to n. If none of the subdiagonal elements are negligible, ℓ is taken to be 0. The following criterion is used

$$|a_{\ell, \ell-1}| \le \varepsilon (|a_{\ell-1, \ell-1}| + |a_{\ell, \ell}|).$$

This criterian examines whether a ℓ , ℓ - 1 is negligible compared to the local diagonal elements.

On each PE $\ell,$ the following computations are simultaneously performed:

$$f(\ell) \equiv |a_{\ell}, \ell - 1| - \epsilon (|a_{\ell} - 1, \ell - 1| + |a_{\ell}, \ell|)$$

for $\ell = 1, 2, ..., n$.

If $f(\ell)$ is negative, 1 is placed in ℓ th bit of the ACAR. Then searching is made for the lowest bit of the ACAR which contains 1. For example, in the following case:

l is set to be 20.

Then test is made if $\ell = n$ or $\ell = n - 1$. If $\ell = n$, one eigenvalue is found in the place (n, n) and the matrix is deflated by 1, and n is decreased by one. In the case that $\ell = n - 1$, two eigenvalues are found as the eigenvalues of the bottom-right hand corner 2 x 2 submatrix. Then two columns and rows are deflated and n is decreased by 2.

5.2 Shifts of origin

The shifts of origin at each stage are taken to be the two roots, s_k and s_{k+1} , of the 2 x 2 matrix in the bottom right-hand corner of the current A_k . This gives

and
$$s_k + s_{k+1} = a_{n-1}, n-1 + a_{n}, n$$

 $s_k + s_{k+1} = a_{n-1}, n-1 + a_{n}, n$

$$s_k + s_{k+1} = a_{n-1}, n-1 + a_{n}, n$$

$$s_k + s_{k+1} = a_{n-1}, n-1 + a_{n}, n$$

$$s_k + s_{k+1} = a_{n-1}, n-1 + a_{n}, n$$

$$s_k + s_{k+1} = a_{n-1}, n-1 + a_{n}, n$$

In some rare cases, the process fails to converge with these shifts of origin. An example of such failure is provided by matrices of the type:

$$\begin{bmatrix}
0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 1
\end{bmatrix}$$

Here the shifts of origin, given in (4), are both zero, and since the matrix is orthogonal, it is invariant with respect to the QR transformation without shifts. However, if one iteration is performed with any shifts of origin which are loosely related to the norm of the matrix, the convergence is very rapid. Therefore in the case where ten iterations do not produce an eigenvalue, the usual shifts s_k and s_{k+1} are replaced by shifts defined by

$$s_k + s_{k+1} = 1.5 (|a_n, n-1| + |a_{n-1}, n-2|).$$

 $s_k s_{k+1} = (|a_n, n-1| + |a_{n-1}, n-2|)^2$
(5)

This strategy is used again after 20 unsuccessful iterations. If 30 unsuccessful iterations are needed then a failure indication is given.

In this program, ITS is the name of an ADB where the iteration count is stored. When ITS \pm 10, 20, we form $S = s_k + s_{k+1}$ and $Y = s_k s_{k+1}$ on a PE n according to (4) and store in ADB's. When ITS \pm 10 or 20, scheme (5) is used for computing S and Y. If ITS \pm 30, it is assumed that this algorithm fails to produce eigenvalues. As a result, only eigenvalues computed prior to this point are given in WR and WI.

5.3 Search for two consecutive small subdiagonal elements

After determining ℓ , (5.1), the submatrix in the rows ℓ to n are examined to see if any two consecutive subdiagonal elements are small enough to work with an even smaller submatrix. To test if we are to start at the row m, we compute the elements p_m , q_m and r_m such that

$$p_{m} = a_{mm}^{2} - a_{mm} (s_{k} + s_{k+1}) + s_{k}s_{k+1} + a_{m,m+1}a_{m+1,m}$$

$$q_{m} = a_{m+1,m} (a_{mm} + a_{m+1,m+1} - s_{k} - s_{k+1})$$

$$r_{m} = a_{m+2,m+1}a_{m+1,m}$$
(6)

The criterion applied is

$$\begin{vmatrix} a_{m, m-1} & (|q_{m}| + |r_{m}|) \\ \leq \epsilon & |p_{m}| & (|a_{m+1, m+1}| + |a_{m, m}| + |a_{m-1, m-1}|) \end{vmatrix}$$
(7)

where we test whether or not the elements which appear in the positions (m+1, m), (m+2, m+1) are negligible compared with the three local diagonal elements a_{m+1} , m+1, m,m and a_{m-1} , m-1.

Here we take m to be the largest integer $(\geq l)$ for which condition (6) is satisfied.

For this computation, the mode bits are turned on for PE ℓ through PE n. The p_m , q_m and r_m for $m=\ell,\ell-1,\ldots$, n are computed according to (6) on all PE's whose mode bits are turned on, and comparison is made to see whether (7) is satisfied. If (7) is satisfied on PE m, 1 is placed in the mth bit of the ACAR. Then the search is made for the lowest bit of the ACAR which contains 1, and m is set equal to this bit number. If no 1 is found in the ACAR, m is taken to be ℓ .

5.4 Double QR-transformation

 A_{k+2} is computed by applying the QR-double transformation to A_k in such a way that $A_{k+2}=N_n^*$ N_m^* A_k N_m N_n

where
$$N_{i}^{*} = I - \frac{U_{i}U_{i}^{*}}{2K_{i}^{2}}$$
 and $U_{i} = (p_{i} + t_{i}, q_{i}, r_{i}, 0 \dots 0)$.

Here

$$p_{i} = a_{ii}^{2} - a_{ii} (s_{k} + s_{k+1}) + s_{k} s_{k+1} + a_{i,i+1} a_{i+1,i}$$

$$q_{i} = a_{i+1,i} (a_{ii} + a_{i+1,i+1} - s_{k} - s_{k+1})$$

$$r_{i} = a_{i+2,i+1} a_{i+1,i}$$
for $i = m$

and

$$p_{i} = a_{i,i-1} + t_{i},$$
 $q_{i} = a_{i+1}, i-1$ and $r_{i} = a_{i+2}, i-1$ for $i \neq m$.

t and 2K² are defined as

$$t_{i} = \pm \sqrt{p_{i}^{2} + q_{i}^{2} + r_{i}^{2}}$$

$$2K_{i}^{2} = t_{i}^{2} + p_{i}t_{i}.$$

Row modification:

For i = m, m + 1, . . . , n, the elements of $N_i^* A_k^{(i)} \equiv N_i^* (N_{i-1} \cdot . . . N_m^* A_k N_m \cdot . . N_{i-1})$ are different from those of $A_k^{(i)}$ in only three rows, i.e., ith, (i + 1)th and (i + 2)th rows. These new elements are computed in the following way with the elements of $A_k^{(i)}$ denoted by $a_{h,j}$:

(i,j) - element =
$$a_{ij}$$
 - $[(p_i \pm t_i)a_{ij} + q_i a_{i+1,j} + r_i a_{i+2,j}] \frac{1}{t_i}$
(i+1,j) - element = $a_{i+1,j}$ - $[(p_i \pm t_i)a_{ij} + q_i a_{i+1,j} + r_i a_{i+2,j}] \frac{q_i}{2K_i^2}$
(i+2,j) - element = $a_{i+2,j}$ - $[(p_i \pm t_i)a_{ij} + q_i a_{i+1,j} + r_i a_{i+2,j}] \frac{r_i}{2K_i^2}$
for $j = i, i + 1, \dots, n$

In the actual computation, t_i and $2K_i^2$ are first computed and then p_i , q_i and r_i are found and stored in ADB's. The mode bits of PE's which contain $a_{i,i}$, $a_{i,i+1}$, \cdots , $a_{i,n}$ are turned on and $c_i \equiv (p_i + t_i)a_{ij} + q_ia_{i+1,j} + r_ia_{i+2,j}$ are computed on these PE's. The computation of new elements

$$(i,j) - \text{element} = a_{i,j} - \frac{c_i}{t_i}$$

$$(i,j+1) - \text{element} = a_{i,j+1} - \frac{c_i q_i}{2K_i^2}$$

$$(i,j+2) - \text{element} = a_{i,j+2} - \frac{c_i r_i}{2K_i^2}$$

are then performed.

Column Modification:

Similarly $(N_i^*A_k^{(i)})N_i$ is computed from $N_i^*A_k^{(i)}$ for $i=m,\ m+1$, . . . , n in the following way where the element of matrix $N_i^*A_i^{(k)}$ are denoted as $a_{i,h}$:

$$(j,i) - \text{element} = a_{ji} - \left[(p_i + t_i)a_{ji} + q_i a_{j,i+1} + r_i a_{j,i+2} \right] \frac{1}{t_i}$$

$$(j,i+1) - \text{element} = a_{j,i+1} - \left[(p_i + t_i)a_{ji} + q_i a_{j,i+1} + r_i a_{j,i+2} \right] \frac{q_i}{2K_i^2}$$

$$(j,i+2) - \text{element} = a_{j,i+2} - \left[(p_i + t_i)a_{ji} + q_i a_{j,i+1} + r_i a_{j,i+2} \right] \frac{r_i}{2K_i^2}$$

$$\text{for } j = \ell, \dots, \text{ min } [i+3,n].$$

As in the row modification, $c_i' = (p_i + t_i)^a_{ji} + q_i^a_{j,i+1} + r_i^a_{j,i+2}$ are computed on the PE's which contain a_{ji} for j from ℓ through min [i + 3, n], then the computations of new (j,i) - element, (j, i + 1) - element and (j, i + 2) - element are performed on the corresponding PE's.

5.5 Computation of eigenvalues

The eigenvalues are calculated as the last step of program after $a_{i+1,i}$ or $a_{i,i-1}$ $a_{i+1,i}$ become negligibly small for all 0 < i < n-2. At each

time when the matrix is deflated by 2, 1 is placed in position n of ADB named SOLV. If the transformation is carried out successfully, SOLV looks like the following,

Here, the eigenvalues we are looking for are a_{00} , a_{33} , a_{44} , a_{55} , a_{88} , $a_{11,11}$, . . . , $a_{61,61}$ and eigenvalues of the following 2 x 2 matrices:

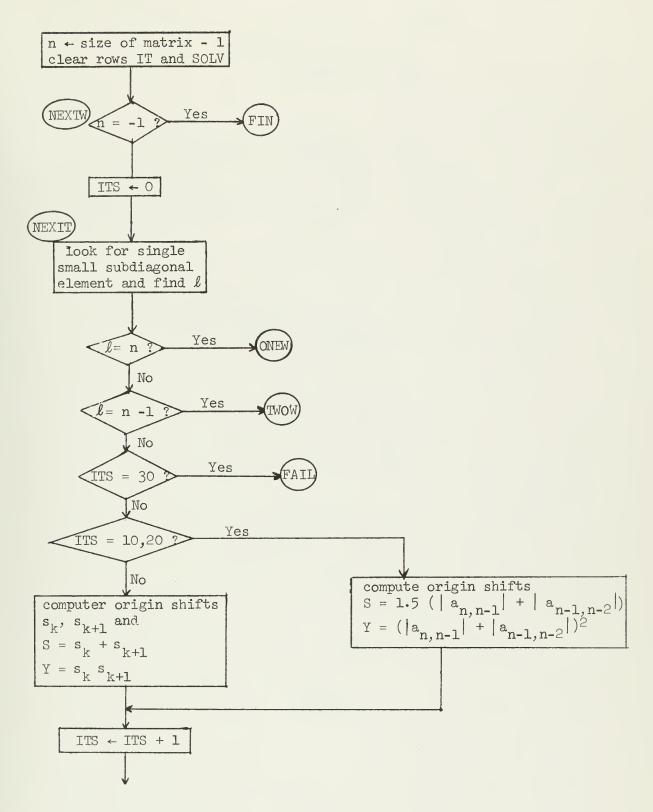
These eigenvalues can be calculated simultaneously on the corresponding PE's.

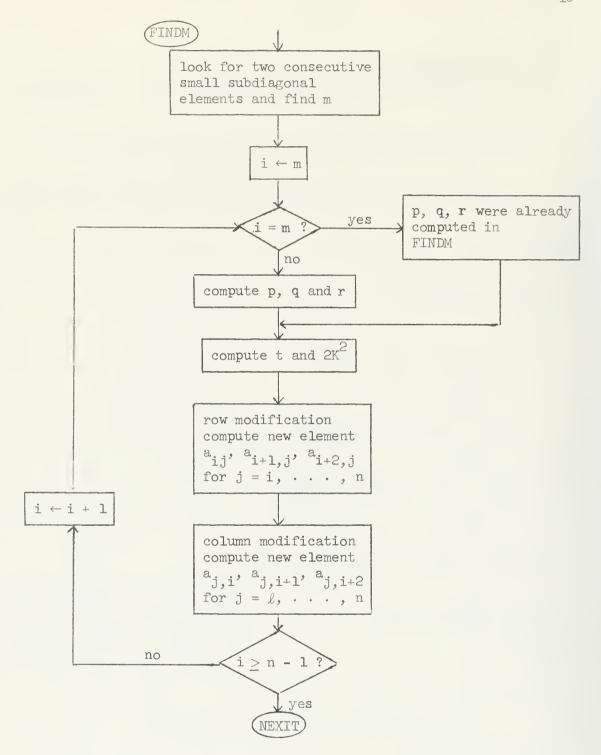
5.6 The number of iteration required

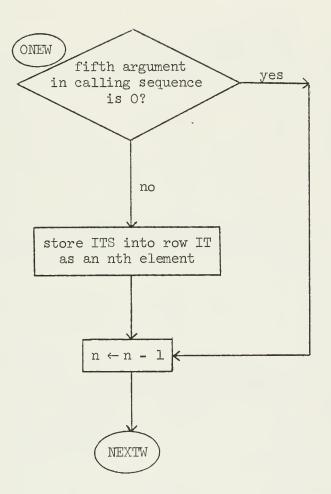
After each deflation, the number of iterations required to find each eigenvalue (or two eigenvalues) appears in ADB named ITS. This is placed as the nth element of the row vector specified by the user as the fifth parameter in the calling sequence. If this parameter is specified as 0, the number of iterations is not stored anywhere.

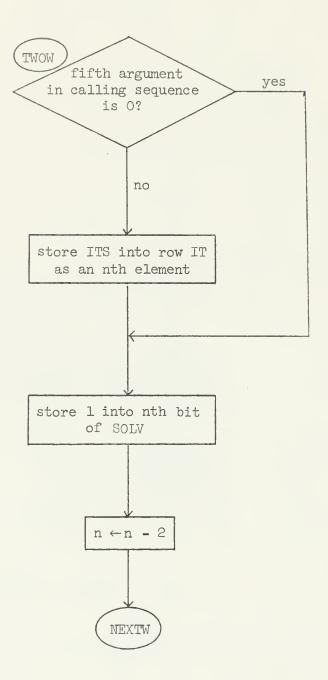
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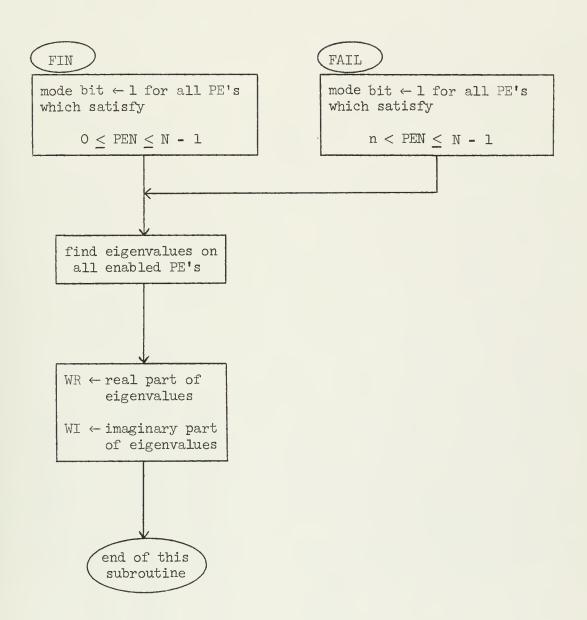
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\$CO\$ 40.NINTUJB 11. CONTSB		HO(3); E OR "E; I AND E;	es Let es	EN E	8 × × 0 (1); 8 × 1 (1); E OR E; • × 1	**************************************	\$41 E OR =F1 \$xo11	m or	E OR E; +0(3);	######################################
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13. ABSTRACT

None

11. SUPPLEMENTARY NOTES

The implementation of QR-algorithm on ILLIAC IV is described. An ASK subroutine for computing all eigenvalues of a real Hessenberg matrix of order less than or equal to 64 by this algorithm is attached. transformation consists of the decomposition of the matrix \boldsymbol{A}_{k} into the product of a unitary matrix Q_k and an upper triangular matrix R_k , and forming A_{k+1} by post-multiplying R_k by Q_k , where A_1 = A is the original matrix. All eigenvalues are either isolated on the diagonal or are eigenvalues of a 2 x 2 diagonal submatrix as $k \rightarrow \infty$.

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